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(54) **AUGMENTED CLASSICAL LEAST SQUARES MULTIVARIATE SPECTRAL ANALYSIS**

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(58) **Field of Search** .............................. 702/18, 22–28, 702/30, 76, 85, 181, 189–190, 196–199; 250/339.09, 339.08, 339.12, 559.1, 573

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(57) **ABSTRACT**

A method of multivariate spectral analysis, termed augmented classical least squares (ACLS), provides an improved CLS calibration model when unmodeled sources of spectral variation are contained in a calibration sample set. The ACLS methods use information derived from component or spectral residuals during the CLS calibration to provide an improved calibration-augmented CLS model. The ACLS methods are based on CLS so that they retain the qualitative benefits of CLS, yet they have the flexibility of PLS and other hybrid techniques in that they can define a prediction model even with unmodeled sources of spectral variation that are not explicitly included in the calibration model. The unmodeled sources of spectral variation may be unknown constituents, constituents with unknown concentrations, nonlinear responses, non-uniform and correlated errors, or other sources of spectral variation that are present in the calibration sample spectra. Also, since the various ACLS methods are based on CLS, they can incorporate the new prediction-augmented CLS (PACLS) method of updating the prediction model for new sources of spectral variation contained in the prediction sample set without having to return to the calibration process. The ACLS methods can also be applied to alternating least squares models. The ACLS methods can be applied to all types of multivariate data.

**10 Claims, 25 Drawing Sheets**

## Concentration-Residual Augmented CLS